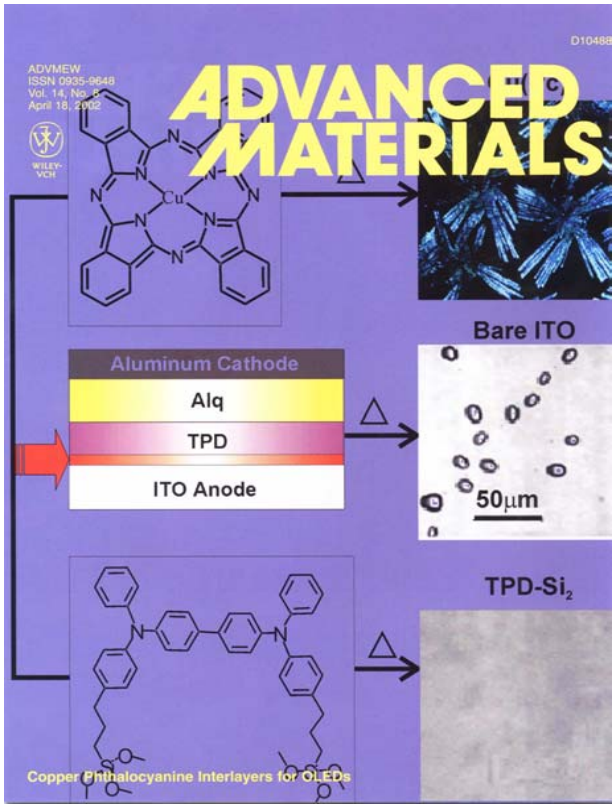
ORGANIC LED ADVANCES REQUIRE CROSSING DISIPLINES

Chemistry ⟷ Materials Science ⟷ Physics

Synthesis ⟷ Processing ⟷ Measurements ⟷ Theory

Academia ⟷ National Labs ⟷ Industry



Microdisplay

Computer Wristwatch

TEAMWORK!

Northwestern-MRSEC

NSLS
National Synchrotron Light Source

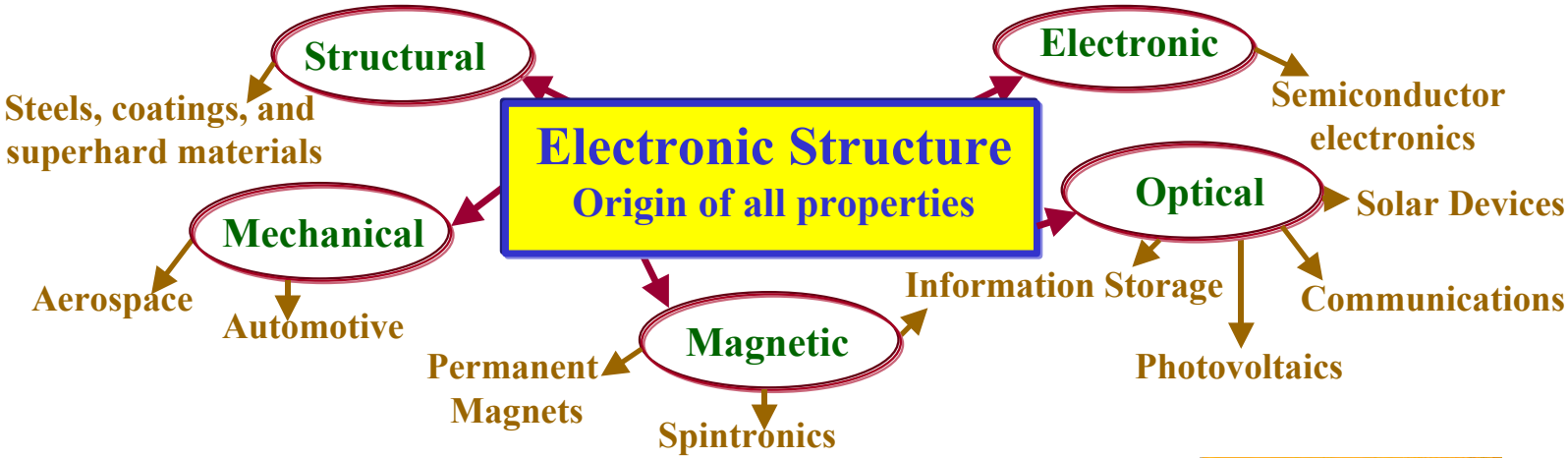
USDC

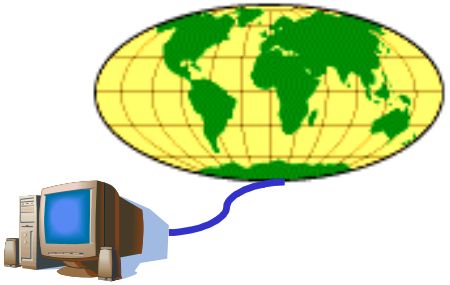
Explanation

Future household and workplace tools and instruments will have an embedded "information appliance" containing a durable, high-brightness, energy-efficient, high resolution display module. Organic Light-emitting diodes (OLEDs) offer great promise in this arena and have stimulated intense worldwide academic and industrial research efforts, driven by such unique applications (including microdisplays and computer wristwatches). A multidisciplinary research team in the Northwestern University MRSEC, led by Prof. T. J. Marks and involving both national laboratories and the U.S. Display Consortium is striving to understand fundamental aspects of OLED charge injection, radiative electron-hole recombination, and failure modes through the designed synthesis, evaluation, and theoretical modeling of self-assembled OLED nanostrustures and interfaces.

Computational Materials Science

Simulation / Modeling → Assisted materials design





International Collaborations
Virtual Computer Laboratory
Encompasses 10 countries

Training & Human Resources Development

Information Dissemination

NU-MRSEC

Computational Materials Science is a new discipline devoted to understanding complex phenomena over a large range of length and time scales. Modeling/simulation can be considered as "experimental theory" or "theoretical experiments."

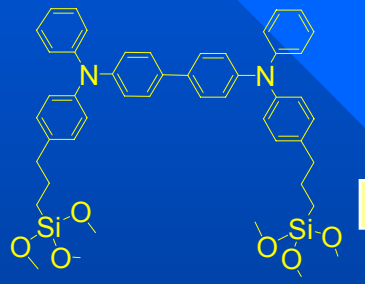
All properties of materials have their origin in the **electronic structure**. Thus, for treating complex materials and their properties, it is essential to employ the most powerful and precise first principles density functional (and beyond) methods to solve this many-body problem, namely the full-potential linearized augmented plane wave method (FLAPW). Now embodied in sophisticated computer programs with many functionalities we have developed, the method is universal in that it can treat all materials and properties from first principles. Some examples of these properties, and their impact on various industries and applications, are given in the schematic diagram above.

An essential component of our work is access to powerful computational facilities which allow us to have **active international collaborations** with researchers and their students in Germany, Switzerland, Italy, Russia, Korea, Japan, China, Taiwan, and Bolivia. This constitutes a **virtual computer laboratory** bringing hardware and software together to solve complex materials problems and to provide training and human resources development. We are also actively engaged in **information dissemination** through the Journal of Magnetism and Magnetic Materials, the premier journal in magnetism, of which A. J. Freeman is the Founding Editor and Editor-in-Chief.

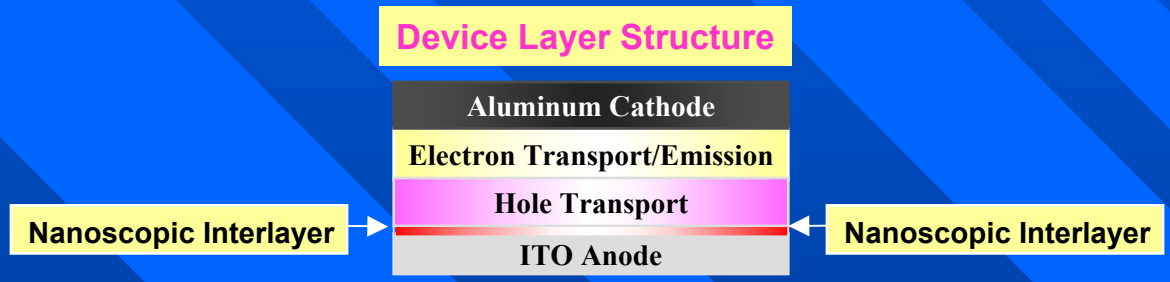
ORGANIC LEDS: FACE OF THE DIGITAL ECONOMY

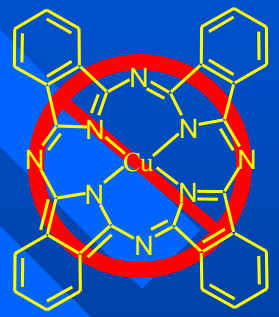
UNIQUE CHARACTERISTICS OF SOFT ELECTRONIC MATERIALS

SELF-ASSEMBLED NANOSCOPIC INTERLAYERS FOR ENHANCED ENERGY EFFICIENCY AND DURABILITY



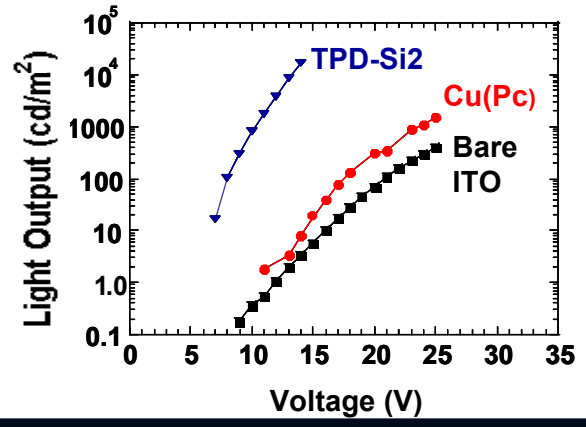
Self-Assembled TPD-Si_2
(Stabilizes Interface)



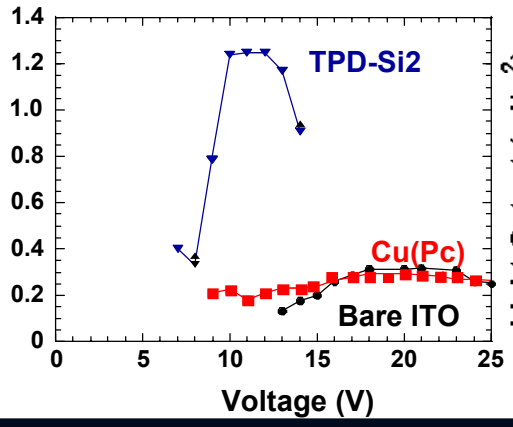


Cu(Pc)
(Industry Standard)

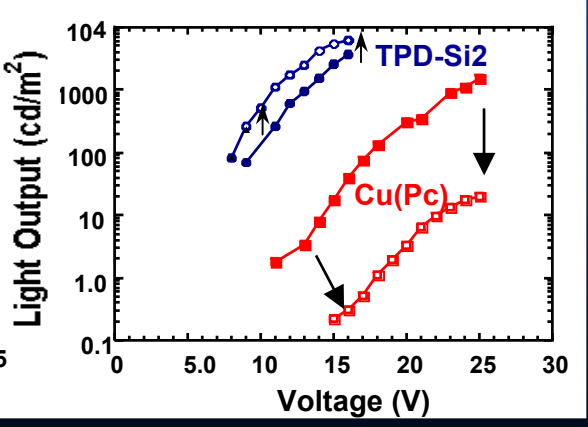
Electroluminescent Response



External Quantum Efficiency



Thermal Stress Effects on EL Response

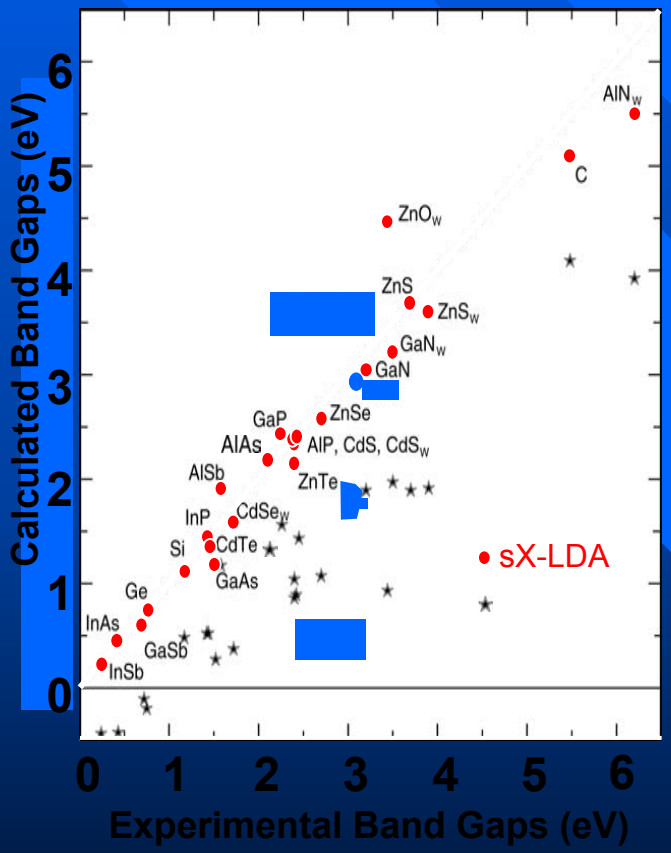


NU-MRSEC T. Marks M. Ratner P. Dutta

Recent research at Northwestern U. shows that the integrity and charge injection characteristics of the interface between the inorganic anode (usually tin-doped indium oxide—ITO) and the organic hole transport layer in organic light-emitting diodes (OLEDs) can be tuned at the nanoscale by self-assembly of appropriately designed aromatic structures. Typical OLED hole transport materials are found to undergo *catastrophic decohesion* on bare ITO, leading to device failure under mild thermal stress. In contrast, self-assembled arylamine interfacial layers prevent decohesion, impart significant OLED thermal robustness, and enhance charge injection efficiency by ~ 10^3x. The commonly used ITO buffer layer, copper phthalocyanine (Cu(Pc)), actually retards charge injection and nucleates deleterious crystallization of the hole transport layer. Optimizing hole and injection characteristics by nanoscale interfacial engineering leads to robust OLEDs with light outputs as high as 100,000 cd/m^2, forward external quantum efficiencies as high as 5%, and power efficiencies as high as 17 L/W.

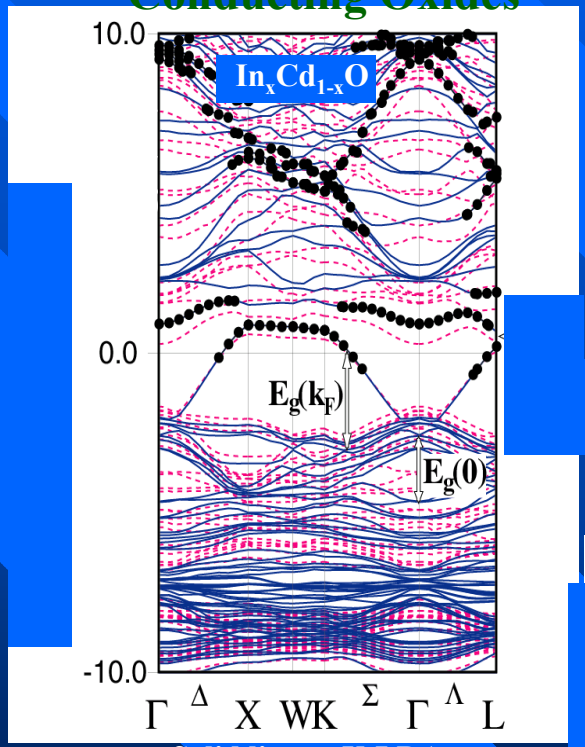
Computational Materials Science for Applications

Band Gap Engineering



Geller, Wolf, Picozzi, Continenza, Asahi, Mannstadt, Freeman, Wimmer, Appl. Phys. Lett. 79, 368 (2001)

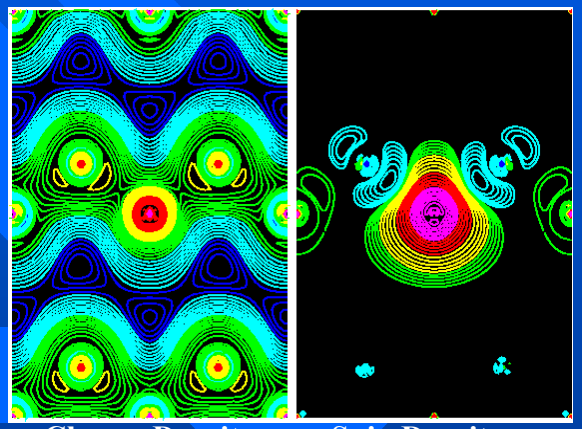
Transparent Conducting Oxides



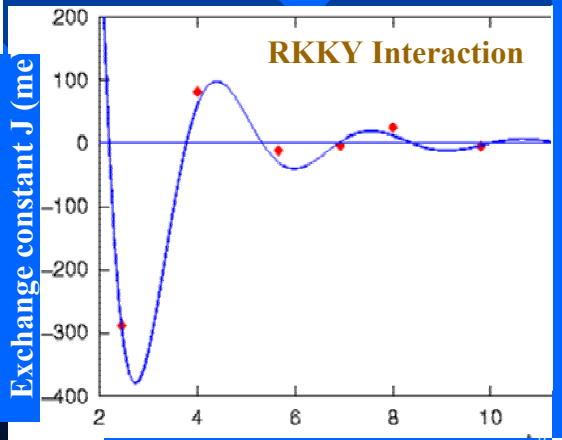
Solid lines: sX-LDA
Dashed lines: LDA
Eg(k_F): 3.19 eV (sX)
3.15 eV (exp)

A.Wang, J.R. Babcock, N.L. Edleman, A.W.Metz, M.A. Lane, R. Asahi, V.P. Dravid, C.R. Kannewurf, A.J. Freeman, T.J. Marks PNAS, 98, 7113 (2001)

Magnetic Semiconductors



Charge Density **Spin Density**



Y.J. Zhao and A.J. Freeman (unpublished 2002)

NU-MRSEC

Computational Materials Science Applications are today numerous and cover many areas of materials research and applications. Here we give three examples which demonstrate our modern forefront capabilities for treating complex issues involving electronic structure determinations. The figure on the left demonstrates the success of our fully first principles calculations with the screened exchange - local density approximation (sX-LDA), given as (●), in overcoming the well-known failure of the LDA, given as (★), for determining excited state properties like band gaps, band offsets, etc. in semiconductors and thus provides **band gaps with engineering accuracy** for use in designing photovoltiacs, solar devices, etc. (Note the totally wrong negative band gaps shown for InSb, InAs, GaSb, and Ge.)

Materials having high electrical conductivity and optical transparency will be essential for next generation flat-panel displays, photovoltiacs, organic light emitting diodes, energy-efficient windows and a host of other opto-electronic technologies. The middle figure shows recent accomplishments in understanding the new **transparent conducting oxide**, $In_xCd_{1-x}O$ films, discovered and developed in our Northwestern University MRSEC. The FLAPW sX-LDA band structure results give a band gap in excellent agreement with experiment, small conduction electron effective masses of CdO, a dramatic Burstein-Moss shift of the band gap with doping, a hybridization gap caused by extensive Cd 5s and In 5s mixing and provides insight into criteria for optimizing TCO film properties.

The attractive idea of manipulating the spin of the electron, in addition to its charge, as an additional degree of freedom, has recently stimulated intense interest in the field named magneto-electronics or ”spintronics” employing newly discovered **ferromagnetic semiconductors** - with potential advantages of increased data processing speed, non-volatility, decreased power consumption and increased integration densities compared with conventional semiconductor devices. We have employed our first principles FLAPW calculations to understand the origin of ferromagnetism in magnetic semiconductors and to predict a new class of materials (based on the chalcopyrite structure) with a higher Curie temperature. The figures at the right show the charge and spin density distributions determined for Mn-doped GaAs and the calculation of the exchange interaction vs. Mn-Mn distance in a large 64 atom supercell, Mn_2Ge_{62}, which surprisingly shows Ruderman – Kittel – Kasuya – Yoshida (RKKY) behavior.